Using MaxSAT for Efficient Explanations of Tree Ensembles

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February 22 – March 1, 2022 | **AAAI**

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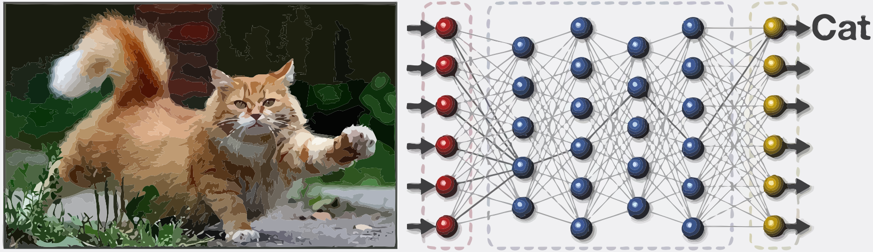
Formal eXplainable AI

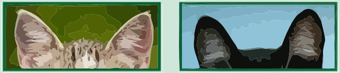
Machine Learning System



This is a cat.

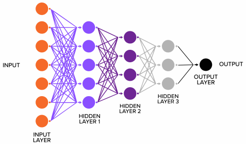
Current Explanation

This is a cat:
- It has fur, whiskers, and claws.
- It has this feature:



XAI Explanation

Why? Status quo...

	A parrot 	Machine learning algorithm 
Learns random phrases	✓	✓
Doesn't understand s**t about what it learns	✓	✓
Occasionally speaks nonsense	✓	✓

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abductive explanation $\mathcal{X}$

$$\forall(\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in \mathcal{X}} (x_j = v_j) \rightarrow (\tau(\mathbf{x}) = \mathbf{c})$$

Formal abductive explanations

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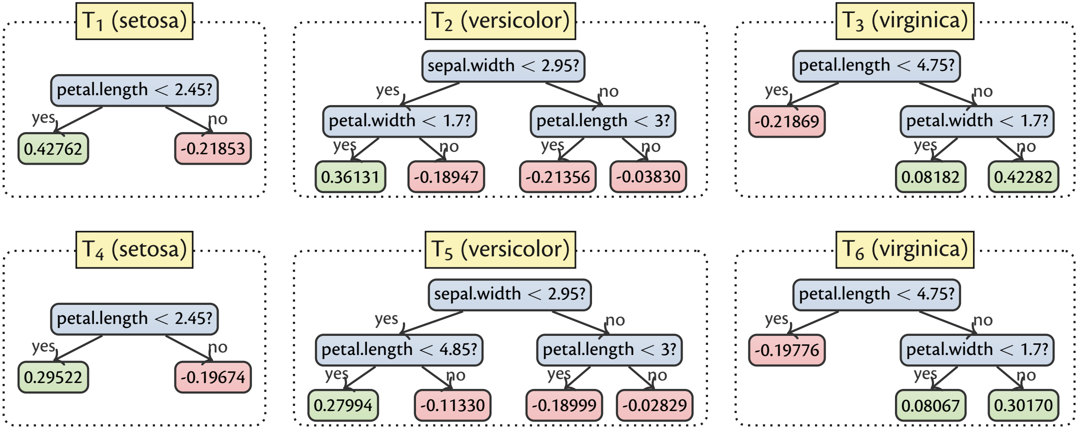
abductive explanation $\mathcal{X}$

"why prediction c?"

$$\forall(\mathbf{x} \in \mathbb{F}). \bigwedge_{j\in\mathcal{X}}(x_j = v_j) \to (\tau(\mathbf{x}) = \mathbf{c})$$

because of features of $\mathcal{X}$**!**

Abductive explanations for tree ensembles



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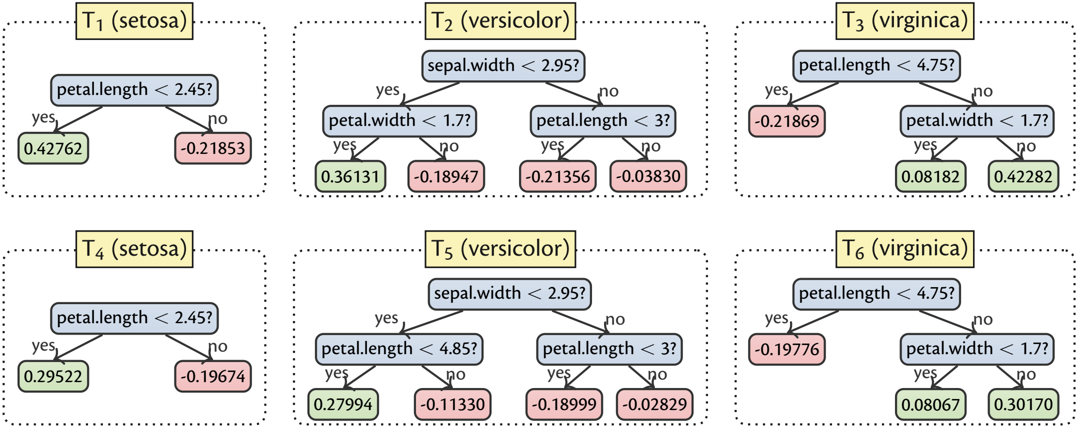

- $w(\mathbf{x}, c) = \sum_{j \in \{0,\ldots,n-1\}} \mathcal{T}_{Kj+c}(\mathbf{x}),\ c \in [K]$
- $\tau(\mathbf{x}) = \arg\max_{c \in [K]} w(\mathbf{x}, c)$

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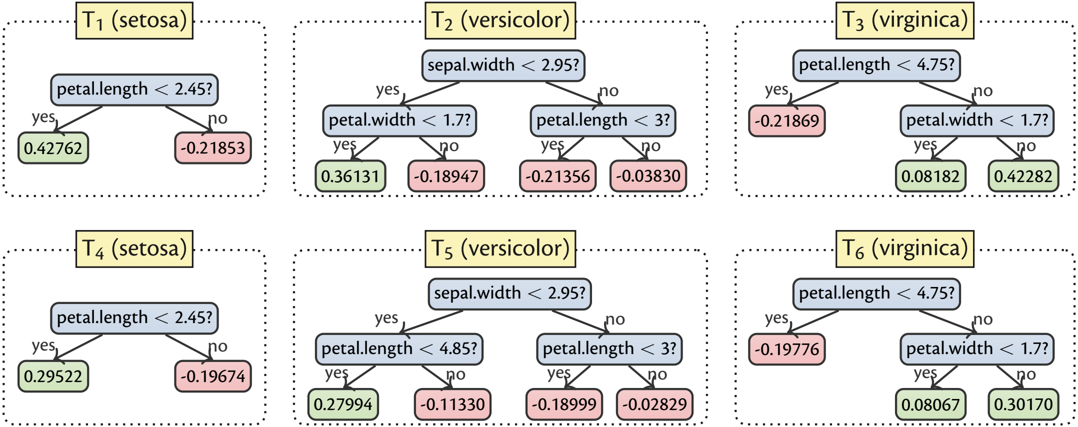

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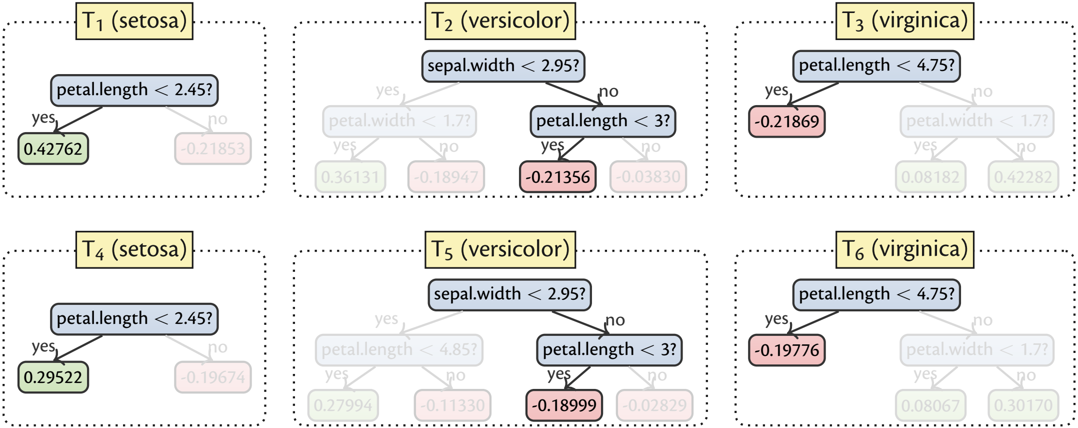

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$(\text{sepal.length} = 5.1) \land (\text{sepal.width} = 3.5) \land (\text{petal.length} = 1.4) \land (\text{petal.width} = 0.2)$

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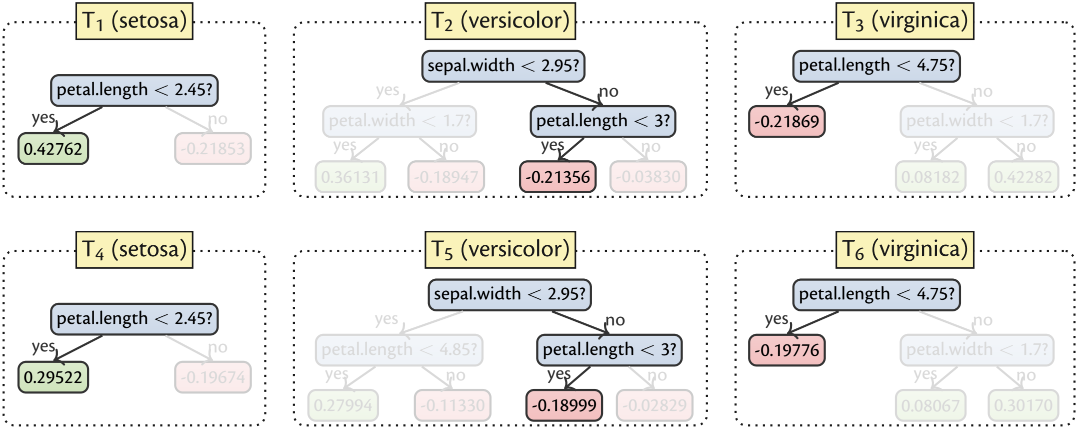

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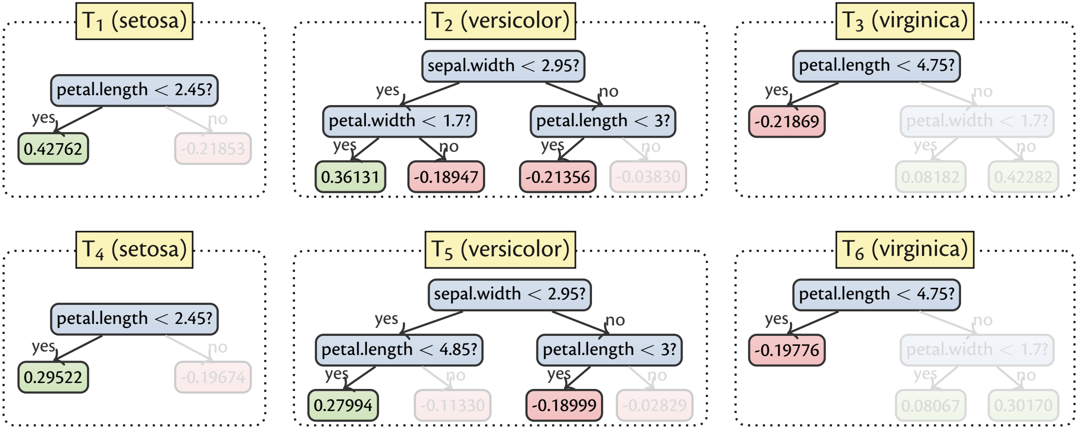

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Formal explanations with MaxSAT

Overview of the approach

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- **reach logic, can handle *linear constraints***

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the devil is in the details

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$\mathcal{F}$ — **set of features** $\forall_{j \in \mathcal{F}}\ D_j$ — **domain of feature j** $\mathfrak{E}$ — **tree ensemble**

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see paper for details

“Optimizing” model predictions

AXp condition for $\mathcal{X}$

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even to represent in propositional logic!

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maximize	$\mathcal{S}_{i,\iota} = \sum_\iota - \sum_i$
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$\mathcal{X}$ is not AXp if $\mathcal{S}^*_{i,\iota} \geqslant 0$

maximize $\mathcal{S}_{i,\iota} = \sum_\iota - \sum_i$

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weighted soft clauses + propositional variables only

multiple calls to a MaxSAT solver with varying assumptions $\mathcal{X}$

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the need for incremental MaxSAT!

Incrementality in MaxSAT

Function MaxSAT(ϕ, $\mathcal{A}$):

Input: ϕ: Partial CNF formula ($\phi \triangleq \mathcal{H} \wedge \mathcal{S}$)

$\mathcal{A}$: Set of assumption literals

Output: μ: MaxSAT model

```
cost ← 0                                  # initially, cost is 0

𝒞 ← ValidCores(ϕ, 𝒜)                      # get valid unsatisfiable cores

foreach κ ∈ 𝒞:                            # iterate over known cores κ
    cost ← cost + CoreWt(κ)               # add its weight to cost

    ϕ ← Process(ϕ, κ)                     # process κ and update ϕ

while SAT(ϕ, 𝒜) = false:                  # iterate until ϕ gets satisfiable
    κ ← GetCore(ϕ)                        # new unsatisfiable core

    cost ← cost + CoreWt(κ)               # add its weight to cost

    ϕ ← Process(ϕ, κ)                     # process κ and update ϕ

    Record(ϕ, 𝒜, κ)                       # record κ for the future

return GetModel(ϕ)                        # ϕ is now satisfiable
```

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$\mathcal{C} \leftarrow$ ValidCores($\phi, \mathcal{A}$) *# get valid unsatisfiable cores*

foreach $\kappa \in \mathcal{C}$: *# iterate over known cores* κ

  cost $\leftarrow$ *cost* + CoreWt(κ) *# add its weight to cost*

  $\phi \leftarrow$ Process(ϕ, κ) *# process* κ *and update* ϕ

while SAT(ϕ, $\mathcal{A}$) = false: *# iterate until* ϕ *gets satisfiable*

  $\kappa \leftarrow$ GetCore(ϕ) *# new unsatisfiable core*

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  $\phi \leftarrow$ Process(ϕ, κ) *# process* κ *and update* ϕ

  Record($\phi, \mathcal{A}, \kappa$) *# record* κ *for the future*

return GetModel(ϕ) *#* ϕ *is now satisfiable*

MiniSat-like assumptions interface:

- assumptions $\mathcal{A} \triangleq \{ l[\![x_j = v_j]\!] \mid j \in \mathcal{X} \}$

Incrementality in MaxSAT

Function MAXSAT(ϕ, $\mathcal{A}$):

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```
cost ← 0                                   # initially, cost is 0
𝒞 ← ValidCores(ϕ, 𝒜)                       # get valid unsatisfiable cores
foreach κ ∈ 𝒞:                             # iterate over known cores κ
    cost ← cost + CoreWt(κ)                # add its weight to cost
    ϕ ← Process(ϕ, κ)                      # process κ and update ϕ
while SAT(ϕ, 𝒜) = false:                   # iterate until ϕ gets satisfiable
    κ ← GetCore(ϕ)                         # new unsatisfiable core
    cost ← cost + CoreWt(κ)                # add its weight to cost
    ϕ ← Process(ϕ, κ)                      # process κ and update ϕ
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```

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unsatisfiable core reuse:

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$\mathcal{C} \leftarrow \textsc{ValidCores}(\phi, \mathcal{A})$ *# get valid unsatisfiable cores*

foreach $\kappa \in \mathcal{C}$**:** *# iterate over known cores* κ

  cost $\leftarrow$ *cost* $+ \textsc{CoreWt}(\kappa)$ *# add its weight to cost*

  $\phi \leftarrow \textsc{Process}(\phi, \kappa)$ *# process* κ *and update* ϕ

while $\text{SAT}(\phi, \mathcal{A}) = \text{false}$**:** *# iterate until* ϕ *gets satisfiable*

  $\kappa \leftarrow \textsc{GetCore}(\phi)$ *# new unsatisfiable core*

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foreach $\kappa \in \mathcal{C}$: *# iterate over known cores κ*

  cost $\leftarrow$ *cost* + CoreWt(κ) *# add its weight to cost*

  $\phi \leftarrow$ Process(ϕ, κ) *# process κ and update ϕ*

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early termination:

- no need to solve the problem to optimality!

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    cost $\leftarrow$ *cost* $+$ CoreWt(κ) *# add its weight to cost*

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LB on the cost is updated at each iteration

return GetModel(ϕ) *#* ϕ *is now satisfiable*

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early termination:

- no need to solve the problem to optimality!
- no misclassification if *cost* $> \sum_\iota$

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```
cost ← 0                                  # initially, cost is 0
C ← VALIDCORES(φ, A)                      # get valid unsatisfiable cores
foreach κ ∈ C:                            # iterate over known cores κ
    cost ← cost + COREWT(κ)               # add its weight to cost
    φ ← PROCESS(φ, κ)                     # process κ and update φ
while SAT(φ, A) = false:                  # iterate until φ gets satisfiable
    κ ← GETCORE(φ)                        # new unsatisfiable core
    cost ← cost + COREWT(κ)               # add its weight to cost
    φ ← PROCESS(φ, κ)                     # process κ and update φ
    RECORD(φ, A, κ)                       # record κ for the future
return GETMODEL(φ)                        # φ is now satisfiable
```

can over-approximate objective once current level is solved

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early termination:

- no need to solve the problem to optimality!
- no misclassification if *cost* $> \sum_\iota$
- misclassification if over-approximation's objective > 0

Additional heuristic — distance-based stratification

why?

why? — many weighted clauses with unique weights

BLO and diversity-based stratification fail to apply!

why? — many weighted clauses with unique weights

BLO and diversity-based stratification fail to apply!

$$\left| w - \frac{\sum_{(c_i, w_i) \in \mathcal{L}} w_i}{|\mathcal{L}|} \right| < \left| w - \frac{\sum_{(c_j, w_j) \in \mathcal{S} \wedge w_j < w} w_j}{|\{(c_j, w_j) \in \mathcal{S} \wedge w_j < w\}|} \right|$$

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$(\neg t_1, 0.72284)$ $(t_2, 0.41527)$ $(\neg t_3, 0.41645)$ $(t_4, 0.16249)$ $(t_5, 0.72452)$

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$$\mathcal{L}_1 = \{ (t_5, 0.72452) \}$$

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$$\left| w - \frac{\sum_{(c_i,w_i)\in\mathcal{L}} w_i}{|\mathcal{L}|} \right| < \left| w - \frac{\sum_{(c_j,w_j)\in\mathcal{S}\wedge w_j<w} w_j}{|\{(c_j,w_j)\in\mathcal{S}\wedge w_j<w\}|} \right|$$

$(\neg t_1, 0.72284)$ $(t_2, 0.41527)$ $(\neg t_3, 0.41645)$ $(t_4, 0.16249)$ $(t_5, 0.72452)$

$$0.00168 = |0.72284 - 0.72452| < |0.72284 - {}^{(0.41645+0.41527+0.16249)}/_3| = 0.39144$$

$$\mathcal{L}_1 = \left\{ (t_5, 0.72452) \right\}$$

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$(\neg t_1, 0.72284)$ $(t_2, 0.41527)$ $(\neg t_3, 0.41645)$ $(t_4, 0.16249)$ $(t_5, 0.72452)$

$$\mathcal{L}_1 = \left\{ \begin{array}{c} (t_5, 0.72452) \\ (\neg t_1, 0.72284) \end{array} \right\}$$

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$$\left| w - \frac{\sum_{(c_i,w_i)\in\mathcal{L}} w_i}{|\mathcal{L}|} \right| < \left| w - \frac{\sum_{(c_j,w_j)\in\mathcal{S}\wedge w_j<w} w_j}{|\{(c_j,w_j)\in\mathcal{S}\wedge w_j<w\}|} \right|$$

$(\neg t_1, 0.72284)$ $(t_2, 0.41527)$ $(\neg t_3, 0.41645)$ $(t_4, 0.16249)$ $(t_5, 0.72452)$

$0.30723 = |0.41645 - {}^{0.72452+0.72284}/_2| > |0.41645 - {}^{(0.41527+0.16249)}/_2| = 0.12757$

$$\mathcal{L}_1 = \left\{ \begin{array}{c} (t_5, 0.72452) \\ (\neg t_1, 0.72284) \end{array} \right\}$$

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$(\neg t_1, 0.72284)$ $(t_2, 0.41527)$ $(\neg t_3, 0.41645)$ $(t_4, 0.16249)$ $(t_5, 0.72452)$

$$\mathcal{L}_1 = \left\{ \begin{array}{c} (t_5, 0.72452) \\ (\neg t_1, 0.72284) \end{array} \right\} \qquad \mathcal{L}_2 = \left\{ \begin{array}{c} (\neg t_3, 0.41645) \\ \end{array} \right\}$$

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$$\left| w - \frac{\sum_{(c_i,w_i)\in\mathcal{L}} w_i}{|\mathcal{L}|} \right| < \left| w - \frac{\sum_{(c_j,w_j)\in\mathcal{S}\wedge w_j<w} w_j}{|\{(c_j,w_j)\in\mathcal{S}\wedge w_j<w\}|} \right|$$

$(\neg t_1, 0.72284)$ $(t_2, 0.41527)$ $(\neg t_3, 0.41645)$ $(t_4, 0.16249)$ $(t_5, 0.72452)$

$0.00118 = |0.41527 - 0.41645| < |0.41527 - 0.16249| = 0.25278$

$$\mathcal{L}_1 = \left\{ \begin{array}{c} (t_5, 0.72452) \\ (\neg t_1, 0.72284) \end{array} \right\} \qquad \mathcal{L}_2 = \left\{ \begin{array}{c} (\neg t_3, 0.41645) \\ \end{array} \right\}$$

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$(\neg t_1, 0.72284)$ $(t_2, 0.41527)$ $(\neg t_3, 0.41645)$ $(t_4, 0.16249)$ $(t_5, 0.72452)$

$0.25337 = |0.16249 - {}^{0.41527+0.41645}/_2| > |0.16249 - 0| = 0.16249$

$$\mathcal{L}_1 = \left\{ \begin{array}{c} (t_5, 0.72452) \\ (\neg t_1, 0.72284) \end{array} \right\} \qquad \mathcal{L}_2 = \left\{ \begin{array}{c} (\neg t_3, 0.41645) \\ (t_2, 0.41527) \end{array} \right\}$$

Additional heuristic — distance-based stratification

why? — many weighted clauses with unique weights

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Experimental results

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  - **200 randomly selected** instances to explain
    - 3665 individual benchmarks in total

Experimental setup

- **competition tested:**
  - **SMT-based formal explainer**
    - makes calls to **Z3 through PySMT**
    - same explanation quality

[1] `https://github.com/alexeyignatiev/xreason/`

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- **prototype**[1]
  - MaxSAT-based
    - **same code base** as in the SMT-based variant
    - applies **incrementally extended** **RC2**
    - makes calls to Glucose 3 through PySAT

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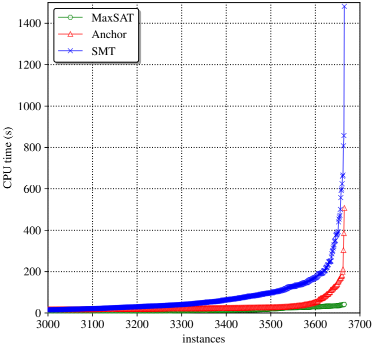
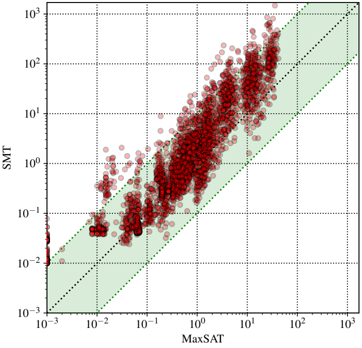
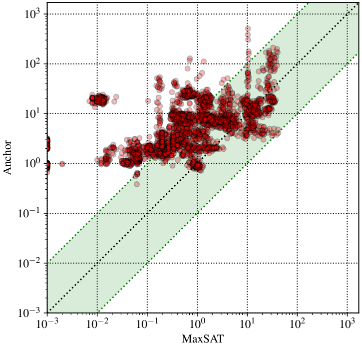
Experimental results



all three competitors



MaxSAT vs. SMT



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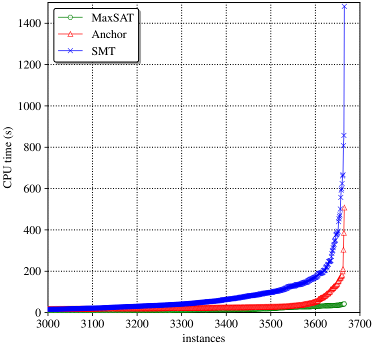

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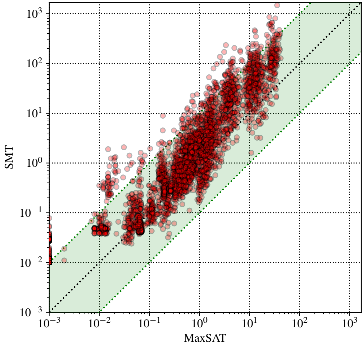

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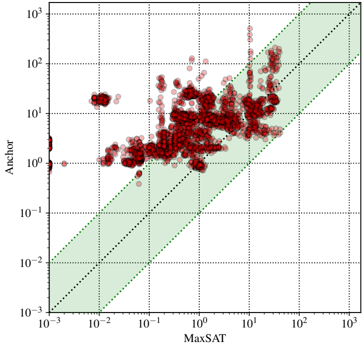

MaxSAT vs. Anchor

up to 2 orders of magnitude performance improvement

more robust than SMT and Anchor

(see paper for details)

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  - **more applications of incremetal MaxSAT?**

Questions?